What We Claim Is:

1. A composition comprising a polypeptide in crystalline form, wherein the polypeptide is a TNF-α-converting enzyme polypeptide.

2. A composition according to claim 1, wherein the TNF-α-converting enzyme polypeptide comprises the TNF-α-converting enzyme catalytic domain.

3. A composition according to claim 1, wherein the TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the pro and catalytic domains of TNF-α-converting enzyme.

4. A composition according to claim 1, wherein the TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the amino acid residues 1-477 of TNF-α-converting enzyme.

5. A composition according to claim 4, wherein the polynucleotide is substituted such that amino acid residue Ser266 is changed to Ala and amino acid residue Asn542 is changed to Gln, and wherein a second polynucleotide encoding the sequence Gly-Ser-$(His)_6$ is fused to the C-terminus.

6. A composition according to claim 1, further comprising a binding partner suitable for co-crystallization with the TNF-α-converting enzyme polypeptide.

7. A composition according to claim 6, wherein the binding partner is a hydroxamate-based binding partner.

8. A composition according to claim 6, wherein the binding partner is N-{D,L-2-(hydroxyaminocarbonyl)methyl-4-methylpentanoyl}-L-3-amino-2-dimethylbutanoyl-L-alanine,2-(amino)ethyl amide.

9. A composition according to claim 1, wherein the crystal has a crystal structure diffracting to 2.0 Å.

10. A composition according to claim 1, wherein the crystal is monoclinic.

11. A composition according to claim 1, wherein the unit cell of the crystal comprises four crystallographically independent TNF-α-converting enzyme catalytic domain (TCD) molecules.

12. A composition according to claim 11, wherein the TCD molecules are in an asymmetric unit.

13. A composition according to claim 1, wherein the crystal is of monoclinic space group $P2_1$ and the cell has the constants a=61.38 A, b=126.27 A, c=81.27 A, and β=107.41°.

14. A composition according to claim 1, wherein the polypeptide is characterized by the structure coordinates according to Table 1, or a substantial part thereof.

15. A method for crystallizing a TNF-α-converting enzyme polypeptide, comprising:

(A) mixing a solution comprising a TACE polypeptide and a binding partner with a crystallization buffer; and

(B) crystallizing the mixture of step (A) by drop vapor diffusion to form a crystalline precipitate.

16. The method according to claim 15, further comprising:

(C) transferring seeds from the crystalline precipitate formed by the drop vapor diffusion and a crystallization promotor into a mixture of a concentrated solution comprising a TACE polypeptide and binding partner substrate, and a crystallization buffer; and

(D) crystallizing the mixture of step (C) by drop vapor diffusion to form a crystal.

17. The method of claim 15, wherein said crystallization buffer is 0.1M Na Citrate pH 5.4, 20%w/v PEG 4000, and 20% v/v Isopropanol.

18.The method of claim 15 or 16, wherein the binding partner is N-{D,L-2-(hydroxyaminocarbonyl)methyl-4-methylpentanoyl}-L-3-amino-2-dimethylbutanoyl-L-alanine, 2-(amino)ethyl amide.

18. The method of claims 15, wherein crystallization is at a temperature ranging from 4 to 20 degrees Celsius.

19. The method of claim 15, wherein the solution comprising the TACE polypeptide and the inhibitor is at a concentration of about 5 mg/mL to about 12 mg/mL in a buffer.

20. The method of claim 19, wherein the solution comprising a TACE polypeptide and the binding partner is mixed with the crystallization buffer in a 1:1 ratio.

21. A tumor necrosis factor-α (TNF-α)-converting enzyme crystal made by co-crystallizing a TNF-α-converting enzyme polypeptide with a co-crystallization substrate.

22. A computer-readable medium having recorded thereon x-ray crystallographic coordinate data for the catalytic domain of TNF-α converting enzyme, or a portion thereof.

23. A computer-readable medium having recorded thereon the x-ray crystallographic coordinate data set forth in Table 1, or a portion thereof.

24. A computer-readable medium of claim 22, wherein the medium is selected from the group consisting of a floppy disc, a hard disc, computer tape, RAM, ROM, CD, DVD, a magnetic disk, and an optical disk.

25. A computer-readable medium having recorded thereon machine-readable data, wherein the computer-readable medium, when used in conjunction with a machine programmed with instructions for using the data, is capable of generating image signals for depicting a graphical, three-dimensional representation of a TNF-α converting enzyme polypeptide, or portion thereof.

26. A system for studying a TNF-α converting enzyme polypeptide, said system comprising:

(a) a memory capable of storing information representing at least a portion of a TNF-α converting enzyme polypeptide, wherein said memory comprises at least one first-type storage region, including a set of spatial coordinates specifying a location in a three dimensional space, and at least one second-type storage region comprising information representing a characteristic of one of a plurality of amino acids, said second-type storage regions being logically associated with said first-type storage regions in said memory to represent a geometric arrangement of at least one characteristic of said at least a portion of said TNF-α converting enzyme peptide in said three dimensional space;

(b) a processor coupled to said memory to access said first-type storage regions and said second-type storage regions, wherein the processor generates image signals for depicting a visual image representing three dimensional image of said at least one characteristic of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space based on data from said memory; and

(c) a display coupled to said processor to receive said image signals, wherein the display depicts a visual three dimensional image of said at least one characteristic of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space based on said image signals.

27. A system as set forth in claim 26, wherein said image signals include signals for depicting a visual three dimensional image of a ribbon structure of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

28. A system as set forth in claim 26, wherein said image signals include signals for depicting a visual image of a solid model representation of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

29. A system as set forth in claim 26, wherein said image signals include signals for depicting a visual three dimensional image of electrostatic surface potential of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

30. A system as set forth in claim 26, wherein said image signals include signals for depicting a visual three dimensional stereo image of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

31. A system as set forth in claim 26, further comprising:

a storage device capable of storing data representing a geometric arrangement of a characteristic of a composition other than said TNF-α converting enzyme polypeptide; and

an operator interface for receiving instructions from a operator; and wherein said processor is coupled to said storage device and to said operator interface and generates additional image signals for depicting said geometric arrangement of said characteristic of said composition relative to said visual three dimensional image of said at least one characteristic of said at least a portion of said TNF-α converting enzyme polypeptide on said display based on instructions from the operator interface.

32. A system as set forth in claim 31, wherein said storage device is part of said memory.

33. A system as set forth in claim 26, comprising a plurality of first-type and second-type storage regions.

34. A video memory capable of storing information for generating a visual display of at least a portion of a TNF-α converting enzyme polypeptide, said video memory comprising:

(a) at least one first-type storage region, each of said first-type storage regions including a set of spatial coordinates specifying a location in a three dimensional space; and

(b) at least one second-type storage region, each of said second-type storage regions containing information for visually depicting a characteristic of one of a plurality of amino acids; wherein said second-type storage regions are logically associated with said first-type storage regions in said video memory to represent a geometric arrangement of at least one characteristic of said at least a portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

35. A video memory as set forth in claim 34, wherein said second-type storage regions are logically associated with said first-type storage regions in said video memory to represent a geometric arrangement of at least one characteristic of a catalytic domain portion of said TNF-α converting enzyme polypeptide in said three dimensional space.

36. A video memory as set forth in claim 34, wherein said first-type storage regions and said second-type storage regions are regions of a semiconductor memory.

37. A video memory as set forth in claim 34, wherein said first-type storage regions and said second-type storage regions are regions of an optical disk.

38. A video memory as set forth in claim 34, wherein said first-type storage regions and said second-type storage regions are regions of a magnetic memory.

39. A video memory as set forth in claim 34, comprising a plurality of first-type and second-type storage regions.

40. A method of identifying a compound that associates with TNF-α-converting enzyme, comprising:

(A) designing an associating compound for said polypeptide that forms a bond with the TNF-α-converting enzyme catalytic domain based on x-ray diffraction coordinates of a TNF-α-converting enzyme polypeptide crystal;

(B) synthesizing said compound; and

(C) determining the associate capability of said compound with said TNF-α-converting enzyme.

41. The method according to claim 40, wherein said associating compound is an inhibitor, mediator, or other compound that regulates TNF-α-converting enzyme activity.

42. The method of claim 41, wherein said associating compound is a competitive inhibitor, un-competitive inhibitor, or non-competitive inhibitor.

43. The method according to claim 40, wherein the coordinates are the coordinates of Table 1, or a substantial part thereof.

44. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal comprises the TNF-α-converting enzyme catalytic domain.

45. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the pro and catalytic domains of TNF-α-converting enzyme.

46. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide is the expression product of a polynucleotide encoding the amino acid residues 1-477 of TNF-α-converting enzyme.

47. The method of claim 46, wherein the polynucleotide is substituted such that amino acid residue Ser266 is changed to Ala and amino acid residue Asn542 is changed to Gln, and wherein a second polynucleotide encoding the sequence Gly-Ser-$(His)_6$ is fused to the C-terminus.

48. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal is co-crystallized with a binding partner.

49. The method of claim 48, wherein the binding partner is a hydroxamate-based binding partner.

50. The method of claim 48, wherein the binding partner is N-{D,L-2-(hydroxyaminocarbonyl)methyl-4-methylpentanoyl}-L-3-amino-2-dimethylbutanoyl-L-alanine,2-(amino)ethyl amide.

51. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal has a crystal structure diffracting to 2.0 Å.

52. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal is monoclinic.

53. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal has a unit cell comprising four crystallographically independent TNF-α-converting enzyme catalytic domain (TCD) molecules.

54. The method of claim 53, wherein the TCD molecules are in an asymmetric unit.

55. The method of claim 40, wherein said TNF-α-converting enzyme polypeptide crystal is of monoclinic space group $P2_1$ and the cell has the constants a=61.38 Å, b=126.27 Å, c=81.27 Å, and β=107.41°.

56. The method of claim 40, wherein the associating compound is designed to associate with the S1' region of TNF-α-converting enzyme.

57. The method of claim 40, wherein the associating compound is designed to associate with the S1'S3' pocket of TNF-α-converting enzyme.

58. The method of claim 40, wherein the associating compound is designed to incorporate a moiety that chelates zinc.

59. The method of claim 40, wherein the associating compound is designed to form a hydrogen bond with Leu348 or Gly349 of TNF-α-converting enzyme.

60. The method of claim 40, wherein the associating compound is designed to introduce a non-polar group which occupies the S1' pocket of TNF-α-converting enzyme.

61. The method of claim 40, wherein the associating compound is designed to introduce a group which lies within the channel joining S1' - S3' pockets of TNF-α-converting enzyme and which makes appropriate van der Waal contact with the channel.

62. The method of claim 40, wherein the associating compound is designed to form a hydrogen bond with Leu348 or Gly349 on the backbone amide groups of TNF-α-converting enzyme.